Berry's Phase in the Presence of a Stochastically Evolving Environment: A Geometric Mechanism for Energy-Level Broadening

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Abstract

The generic Berry phase scenario in which a two-level system is coupled to a second system whose dynamical coordinate is slowly-varying is generalized to allow for stochastic evolution of the slow system. The stochastic behavior is produced by coupling the slow system to a heat reservoir which is modeled by a bath of harmonic oscillators initially in equilibrium at temperature T, and whose spectral density has a bandwidth which is small compared to the energy-level spacing of the fast system. The well-known energy-level shifts produced by Berry's phase in the fast system, in conjunction with the stochastic motion of the slow system, leads to a broadening of the fast system energy-levels. In the limit of strong damping and sufficiently low temperature, we determine the degree of level-broadening analytically, and show that the slow system dynamics satisfies a Langevin equation in which Lorentz-like and electric-like forces appear as a consequence of geometrical effects. We also determine the average energy level-shift produced in the fast system by this mechanism.

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I. INTRODUCTION

In the 14 years since its discovery, Berry's phase has proven to be a fruitful development in our understanding of the adiabatic limit of quantum mechanics [1]. In his original analysis [2], Berry considered a quantum system with a discrete, non-degenerate energy spectrum whose dynamics is driven by a set of classical parameters $\mathbf{R}(t)$ that vary slowly on the time scale of the quantum system. He showed that when $\mathbf{R}(t)$ was cycled adiabatically through a loop in parameter space, and the quantum system was initially prepared in an eigenstate $|E(0)\rangle$ of the initial Hamiltonian $H(0)$, the quantum system returned to the initial state $|E(0)\rangle$ at the end of the cycle, to within a phase factor $\exp(i\phi)$. This much was in agreement with the quantum adiabatic theorem. What was new was that the phase ϕ contained a contribution ϕ_g whose origin was found to be deeply geometrical [3], and which had been discarded in previous treatments of this theorem. ϕ_g is now referred to as Berry's phase, and is a functional $\phi_g[\mathbf{R}(t)]$ of the loop traced out by $\mathbf{R}(t)$ in parameter space.

Not long after Berry's discovery, it was suggested by Moody et. al. [4] that Berry's phase should be observable in nuclear magnetic resonance. It was argued that Berry's phase would produce a shift in the energy levels of the resonating spin which would alter the observable resonant frequencies. This shift was subsequently observed by Suter et. al. [5]. Berry's phase has also been observed in a number of other experimental settings [1]. For our purposes, though, the NMR context will be the most relevant.

The original Berry scenario was generalized in a number of ways in the years following his discovery [1]. For the purposes of this paper, however, the most interesting development was the elevation of the slowly varying classical parameters $\mathbf{R}(t)$ to the status of dynamical quantum variables [6,7]. The total system now consists of a slow subsystem with coordinates $\mathbf{R}(t)$ coupled to a fast spin-like degree of freedom $\boldsymbol{\sigma}$. The separation of dynamic time scales allows a Born-Oppenheimer treatment of the coupled dynamics. The fast system is again found to develop a Berry phase in those states evolving out of an instantaneous energy eigenstate due to the motion of the slow system. Berry's phase again produces shifts in the fast system energy levels. These shifts are functionals $\delta E[\mathbf{R}(t)]$ of the slow system path $\mathbf{R}(t)$. Geometrical effects also influence the motion of the slow system. They lead to the appearance of gauge fields which act on the motion of the slow system [6–10]. The gauge fields produce Lorentz-like and electric-like forces in the classical equation of motion of the slow system.

In this paper, we examine a generalization of the Born-Oppenheimer scenario in which the slow system is allowed to evolve stochastically. The stochastic behavior is introduced by coupling the slow system to a heat resevoir which we represent by a bath of harmonic oscillators initially in thermal equilibrium at temperature T. At first, all 3 subsystems will be quantum mechanical. Ultimately, we will be interested in the case where the stochastic behavior is classical, so eventually we will take the semiclassical limit of the coupled slow system/heat resevoir dynamics. The fast system remains quantum mechanical throughout. We will examine how the stochastic motion of the slow system influences the Berry phase effects discussed above.

For easy reference, we summarize our principal results. *First*, because the semiclassical motion of the slow system is a random process, the energy-level shifts produced by Berry's phase in the fast system's spectrum will cause these levels to broaden. This can be simply

understood in the following way. Due to the stochastic force acting on the slow system (see below), the boundary conditions imposed on the path $\mathbf{R}(t)$ no longer determine a unique path. Instead, all possible realizations of the random process $\mathbf{R}_i(t)$ must be considered which satisfy the boundary conditions. Each realization $\mathbf{R}_i(t)$ will produce a level-shift $\delta E[\mathbf{R}_i(t)]$ with a probability $P[\mathbf{R}_i(t)]$. Thus all possible shifts in the original energy E are produced, though with differing probabilities. The result is that the original energy level E is broadened out by the stochastic evolution of the slow system, in conjunction with the Berry phase induced level-shifts. We will calculate the average energy shift $\overline{\delta E}$ produced, and the variance associated with the spread of energy shifts about $\overline{\delta E}$, under appropriate restrictions. *Second*, we show that the semiclassical motion of the slow system is governed by a Langevin equation. Geometrical effects are seen to produce the same Lorentz-like and electric-like forces in this equation as were found in the original Born-Oppenheimer scenario in which the slow system evolved deterministically. We are able to determine the probability distribution $P[\mathbf{R}_i(t)]$ which we use to calculate the average energy level-shift and broadening produced in the fast system.

The organization of this paper is as follows. We begin in Section II by reviewing those Berry phase results which are pertinent to the work described in this paper. In Section III we introduce the model system we shall study. In Section IV we set-up a path integral representation of its dynamics. We implement the Born-Oppenheimer approximation, watching carefully for the appearance of Berry's phase. We also integrate out the unobserved reservoir degrees of freedom. This yields an effective description of the slow system dynamics in which only $\mathbf{R}(t)$ enters as a dynamical variable. Although the fast system and the resevoir no longer appear in this effective description explicitly, they do produce a back action on the effective slow dynamics which we obtain while carrying out the above maneuvers. In Section V we take the semiclassical limit of the effective slow system dynamics. We find that the slow system motion is governed by a Langevin equation in which the geometry-induced gauge forces appear. We also obtain the probability distribution governing the random process $\mathbf{R}(t)$. In Section VI we use this probability distribution to set-up a generating function for the moments of the energy-level shift $\delta E[\mathbf{R}(t)]$. We use the generating function to calculate the average energy-level shift and level-broadening, under appropriate restrictions. In Section VII, we summarize our results and make closing remarks. Finally, in an Appendix, we calculate the spectral density for classical Brownian motion; the goal being to determine what restrictions are needed to insure that the stochastic motion of the slow system is adiabatic relative to the fast system.

II. BERRY PHASE PRELIMINARIES

In this section we collect the Berry phase results which are relevant to the work we shall present below. The reader is referred to Ref. [6] for a more detailed presentation.

In the original Berry phase scenario [2], the focus of attention is a quantum system with a discrete, non-degenerate energy spectrum. Its Hamiltonian $H[\mathbf{R}]$ is assumed to depend on a set of classical parameters $\mathbf{R}$ which represent an environmental degree of freedom to which the quantum system is coupled. The environment is assumed to evolve adiabatically. This produces an adiabatic time dependence in the quantum Hamiltonian, $H = H[\mathbf{R}(t)]$. The time dependence of the quantum state $|\psi(t)\rangle$ is determined by solving Schrodinger's

equation using the quantum adiabatic theorem. Towards this end, one introduces the energy eigenstates of the instantaneous Hamiltonian $H[\mathbf{R}(t)]$,

$$H[\mathbf{R}(t)]\,|E[\mathbf{R}(t)]\,\rangle = E[\mathbf{R}(t)]\,|E[\mathbf{R}(t)]\,\rangle \qquad .$$

It is further assumed that the environment is taken adiabatically around a loop in parameter space such that $\mathbf{R}(T) = \mathbf{R}(0)$, and that the quantum system is initially prepared in an eigenstate $|E[\mathbf{R}(0)]\rangle$ of the initial Hamiltonian $H[\mathbf{R}(0)]$. The quantum adiabatic theorem states that, at time t, the quantum system will be found in the state $|E[\mathbf{R}(t)]\rangle$ to within a phase factor,

$$|\psi(t)\rangle = \exp\left[i\gamma_E(t) - \frac{i}{\hbar}\int_0^t d\tau E[\mathbf{R}(\tau)]\right]|E[\mathbf{R}(t)]\rangle \ . \tag{1}$$

The second term in the phase of the exponential is known as the dynamical phase and was already familiar from previous studies of the quantum adiabatic theorem. The first term represents Berry's discovery, and is referred to as Berry's phase,

$$\gamma_E(t) = i\int_0^t d\tau\,\langle E[\mathbf{R}(\tau)]|\frac{\partial}{\partial\tau}|E[\mathbf{R}(\tau)]\rangle \qquad . \tag{2}$$

In the cases where Berry's phase is physically relevant, γ_E is non-integrable: it cannot be written as a single-valued function of $\mathbf{R}$ over all of parameter space. Simon [3] showed that the quantum adiabatic theorem has a line bundle structure inherent in it, and that Schrodinger's equation defines a parallel transport of the quantum state around the line bundle. Berry's phase is the signature that the associated connection has non-vanishing curvature.

Berry's phase has been observed in a number of physical systems [1]. For present purposes, the nuclear magnetic resonance experiments are the most interesting. Moody et. al. [4] pointed out that Berry's phase should alter the observed resonant frequencies in NMR. In particular, if one were examining the resonance associated with the pair of levels E and E', the shift in the resonant frequency $\Delta\omega_0$ would be,

$$\Delta\omega_0 = \frac{\gamma_E(\mathcal{T}) - \gamma_{E'}(\mathcal{T})}{\mathcal{T}} \qquad ,$$

where $\mathcal{T}$ is the period of the oscillating transverse magnetic field $\mathbf{H}_\perp(t)$. The resonant frequency shift occurs because a shift δE is produced in each energy-level E by Berry's phase,

$$\delta E = \frac{\hbar\gamma_E(\mathcal{T})}{\mathcal{T}} \qquad . \tag{3}$$

In the NMR experiments both E and $\dot{\gamma}_E$ were time independent. Since $\gamma_E(\mathcal{T})$ is independent of the parameterization of $\mathbf{R}(t)$, so long as the new parameterization remains adiabatic, eqn. (3) will also be correct when $\dot{\gamma}_E \neq$ *constant*. One simply reparameterizes the time $t \rightarrow t'$ in such a way that $\dot{\gamma}_E(t')$ is time independent.

The above scenario can be generalized. We promote $\mathbf{R}(t)$ from a classical degree of freedom with no dynamics of its own, to a fully-dynamical quantum variable [6,7]. As

above, $\mathbf{R}(t)$ couples to a spin-like degree of freedom $\boldsymbol{\sigma}$. For the remainder of this paper we will assume that $\boldsymbol{\sigma}$ corresponds to a pseudo-spin 1/2. To stay within the context of the quantum adiabatic theorem, we assume that a Born-Oppenheimer treatment of the coupled dynamics is appropriate, and that $\mathbf{R}$ ($\boldsymbol{\sigma}$) is the dynamical variable of the slow (fast) system. The Hamiltonian for the coupled system is taken to be

$$H_{tot} = \frac{\mathbf{P}^2}{2M} + V[\mathbf{R}] - g\mathbf{R}\cdot\boldsymbol{\sigma} \qquad . \tag{4}$$

Here $\mathbf{P}$ is the momentum conjugate to $\mathbf{R}$; $\boldsymbol{\sigma}_i$ are the Pauli matrices; we allow for the possibility of a potential V acting on the slow system; and g is a coupling constant.

In applying the Born-Oppenheimer approximation, one first considers the fast system, treating the slowly-varying $\mathbf{R}$ as fixed. The fast motion is governed by $H_f = -g\mathbf{R}\cdot\boldsymbol{\sigma}$ with eigenstates $|E_\pm(\mathbf{R})\rangle$ and energies $\pm gR$, where $R = |\mathbf{R}|$. In fact, $\mathbf{R}$ varies adiabatically. From the quantum adiabatic theorem we know that when the fast system is prepared initially in the state $|E[\mathbf{R}(0)]\rangle$, its state at time t is given by eqns. (1) and (2), and Berry's phase produces the energy level shift δE given by eqn. (3). The slow dynamics is governed by

$$\begin{aligned} H_{eff} &= \langle E(\mathbf{R})|H_{tot}|E(\mathbf{R})\rangle \\ &= \frac{(\mathbf{P}-\mathbf{A}[\mathbf{R}])^2}{2M} + \Phi\left(\mathbf{R}\right) + E\left(\mathbf{R}\right) \quad . \end{aligned} \tag{5}$$

Here,

$$\mathbf{A}(\mathbf{R}) = i\hbar\langle E(\mathbf{R})|\nabla_{\mathbf{R}}|E(\mathbf{R})\rangle \qquad , \tag{6}$$

and,

$$\Phi(\mathbf{R}) = \frac{\hbar^2}{2}\sum_{i=\pm} g_{ii}(\mathbf{R}) \qquad . \tag{7}$$

From eqns. (2) and (6), we see that $\mathbf{A}[\mathbf{R}]$ is related to Berry's phase: $\hbar\dot{\gamma}_E = \dot{\mathbf{R}}\cdot\mathbf{A}[\mathbf{R}]$. $g_{ij}(\mathbf{R})$ is the quantum metric tensor [6,11] and corresponds to the real part of the quantum geometric tensor T_{ij},

$$T_{ij} = \langle\partial_i E|\left(1 - |E\rangle\langle E|\right)|\partial_j E\rangle \qquad ,$$

where $\partial_i = \partial/\partial R_i$. We see that geometrical effects produce gauge potentials Φ and $\mathbf{A}$ in the effective Hamiltonian that governs the slow dynamics. In the semiclassical limit, the equation of motion for the slow system is [6]

$$M\ddot{\mathbf{R}} = \dot{\mathbf{R}}\times\mathbf{B}[\mathbf{R}] - \nabla_{\mathbf{R}}\left[\Phi[\mathbf{R}] + V[\mathbf{R}] + E[\mathbf{R}]\right], \tag{8}$$

where $\mathbf{B} = \nabla\times\mathbf{A}$. Thus, geometrical effects lead to the appearance of Lorentz-like and electric-like forces that act on the slow system in the semiclassical limit.

This concludes our summary of the Berry phase physics we shall need below.

III. THE MODEL

As mentioned in the Introduction, we would like to explore how the Berry phase physics discussed in Section II is affected by stochastic motion of the slow system. To produce stochastic behavior, we introduce a heat resevoir that couples to the slow system, and which initially is in thermal equilibrium at temperature T. Because the resevoir degrees of freedom are unobserved, they must be traced out of the dynamical description. The result of this operation is that stochastic and frictional forces appear in the dynamics of the slow system.

To produce a tractable model, some restrictions must be placed on the heat resevoir, and on its coupling to the slow system. These restrictions, and the model to which they lead, have been discussed in great detail in the literature [12,13]. Consequently, our discussion here will be brief. The reader is referred to these papers for further discussion.

The first restriction imposed is that the heat resevoir contain an infinite number of degrees of freedom. The idea here is that any energy transferred from the slow system to the infinitely many resevoir degrees of freedom effectively disappears into the resevoir, not to return in any physically reasonable amount of time. The result is dissipation of energy and irreversibility in the motion of the slow system.

The second restriction is that the slow system couple weakly to the individual resevoir degrees of freedom. As such, each resevoir degree of freedom is only weakly disturbed from equilibrium. This restriction allows us to analyze the excitation of the resevoir away from equilibrium using a harmonic approximation [12,13]. Consequently, the resevoir degrees of freedom can be modeled by harmonic oscillators that represent the normal modes of the resevoir.

This combination of restrictions is known to produce stochastic and frictional forces in the semiclassical motion of the slow system once the resevoir has been traced out [14,15]. Because Berry's phase requires the slow system to evolve adiabatically relative to the fast system, we must add a further restriction to insure adiabaticity of the stochastic motion. The essential point is the following. Because of the stochastic force, $\mathbf{R}(t)$ contains fluctuations or noise. The range of frequencies $\Delta\omega$ present in the fluctuations can be determined by examining the spectral density $J_{\mathbf{R}}(\omega)$ of $\mathbf{R}(t)$. In the Appendix we show that, in the semiclassical limit, $J_{\mathbf{R}}(\omega)$ is proportional to the spectral density $J_{\mathbf{F}}(\omega)$ of the stochastic force $\mathbf{F}(t)$. The range of frequencies (bandwidth) present in $\mathbf{F}(t)$ is of order $1/\tau_c$, where τ_c is the correlation time of $\mathbf{F}(t)$. The correlation time is known for our model of the resevoir [15]: $\tau_c = \hbar/\sqrt{6}kT$. Thus the bandwidth $\Delta\omega$ of the random process $\mathbf{R}(t)$ is also of order $1/\tau_c$. We can insure that $\mathbf{R}(t)$ evolves adiabatically if we require that $\hbar\Delta\omega$ be much less than the energy-level spacing of the fast system, $\Delta E = E_+ - E_-$. This is the final restriction we need to impose on the slow system/reservoir dynamics. For example, since $\hbar\Delta\omega \sim \sqrt{6}kT$, we see that when $1\,\mathrm{K} \leq T \leq 100\,\mathrm{K}$, the bandwidth for fluctuations in $\mathbf{R}(t)$ satisfies $10^{-4}\,\mathrm{eV} \leq \hbar\Delta\omega \leq 10^{-2}\,\mathrm{eV}$. Thus if $\Delta E > 0.1\,\mathrm{eV}$, the slow system will evolve adiabatically relative to the fast system, even though its dynamics is stochastic.

Assuming that all 3 of these restrictions are satisfied, the following model Hamiltonian will produce adiabatic stochastic motion of the slow system:

$$H = \left(\frac{\mathbf{P}^2}{2M} + V[\mathbf{R}] \right) - g\mathbf{R}\cdot\boldsymbol{\sigma}$$

$$
+\sum_j \frac{m_j}{2}\left(\dot{\mathbf{Q}}_j^2 - \omega_j^2 \mathbf{Q}_j^2\right)
$$

$$
+\sum_j C_j \mathbf{R}\cdot\mathbf{Q}_j + \mathbf{R}^2 \sum_j \frac{C_j^2}{2m_j\omega_j^2} \quad . \tag{9}
$$

The first term on the right-hand side (rhs) is the non-interacting slow system Hamiltonian H_s. The second term on the rhs is the slow system/fast system interaction Hamiltonian H_{sf}. The third term is the non-interacting resevoir Hamiltonian H_r, and the last two terms give the slow system/resevoir interaction Hamiltonian H_{sr}. m_j and ω_j are the oscillator masses and frequencies, respectively; and C_j are the coupling constants for the slow system/oscillator interactions. These constants are not determined by the model, though they satisfy a constraint [12] that connects them to the friction coefficient η that will appear in the Langevin equation obtained in Section V. The last term on the rhs is a counter-term introduced to insure that $V(\mathbf{R})$ is the potential acting on the slow system in the semiclassical limit.

Having introduced our model, our next task is to set-up a path integral treatment of its dynamics.

IV. DYNAMICS VIA PATH INTEGRALS

In this Section we apply the influence functional formalism of Feynman and Vernon [13] to describe the dynamics of our model. The analysis begins with the density matrix for the composite system (slow system/fast system/resevoir). The essentials of its time development are presented in Section IV A. The Born-Oppenheimer approximation is implemented in Section IV B, and the resevoir degrees of freedom are traced out in Section IV C. The main result of this section will be a path integral representation of the reduced density matrix describing the effective dynamics of the slow system. Geometrical contributions to this effective dynamics appear during implementation of the Born-Oppenheimer approximation; stochastic and dissipative effects enter in when tracing out the resevoir, though this will not become apparent until Section V.

A. Density Matrix Preliminaries

We begin with the density operator $\rho(t)$ of the composite system. Its evolution is given by,

$$
\rho(t) = \exp\left[-\frac{i}{\hbar}\left(t+\frac{\mathcal{T}}{2}\right)H\right]\rho\left(-\frac{\mathcal{T}}{2}\right)\times\exp\left[\frac{i}{\hbar}\left(t+\frac{\mathcal{T}}{2}\right)H\right] . \tag{10}
$$

H is the Hamiltonian for the composite system (see eqn. (9)), and the time evolution begins at $t=-\mathcal{T}/2$.

It proves useful to work in the basis $|\mathbf{x},\,\sigma,\,\mathbf{z}\,\rangle$ in which the slow system is at $\mathbf{x}$, the fast system has pseudo-spin projection σ along $\mathbf{x}$, and the harmonic oscillators have positions $\mathbf{Z} = (\ldots,\mathbf{Z}_j,\ldots)$, where j labels the oscillator degrees of freedom. In this basis, eqn. (10) becomes,

$$\langle\, \mathbf{x}_f, \sigma_f, \mathbf{Q}_f |\, \rho(t)\, | \mathbf{y}_f, \sigma'_f, \mathbf{Z}_f \,\rangle =$$
$$\sum_{\sigma,\sigma'} \int d\mathbf{x}'\, d\mathbf{y}'\, d\mathbf{Q}'\, d\mathbf{Z}'\, \langle \mathbf{x}', \sigma, \mathbf{Q}' | \rho(-\mathcal{T}/2) | \mathbf{y}', \sigma', \mathbf{Z}' \rangle$$
$$\times\, K(\mathbf{x}_f, \sigma_f, \mathbf{Q}_f, t; \mathbf{x}', \sigma, \mathbf{Q}', -\mathcal{T}/2)\, K^*(\mathbf{y}_f, \sigma'_f, \mathbf{Z}_f, t; \mathbf{y}', \sigma', \mathbf{Z}', -\mathcal{T}2). \quad (11)$$

Here,

$$K(\mathbf{x}_f, \sigma_f, \mathbf{Q}_f, t; \mathbf{x}', \sigma, \mathbf{Q}', -\mathcal{T}/2) = \langle \mathbf{x}_f, \sigma_f, \mathbf{Q}_f | \exp\left[-\frac{i}{\hbar} \left(t + \frac{\mathcal{T}}{2} \right) H \right] | \mathbf{x}', \sigma, \mathbf{Q}' \rangle.$$

K^* is the complex conjugate of K and will not be written out explicitly. In Section IV B we will obtain a path integral expression for K.

We must specify an initial condition for the time development. We assume that the resevoir is uncoupled from the slow/fast systems prior to $t = -\mathcal{T}/2$. Thus $\rho(-\mathcal{T}/2)$ factors:

$$\rho\left(-\mathcal{T}/2\right) = \rho_r\left(-\mathcal{T}/2\right)\, \rho_{sf}\left(-\mathcal{T}/2\right) \quad . \quad (12)$$

The resevoir is assumed to be in thermal equilibrium at temperature T initially. Thus the energy-levels of each oscillator degree of freedom are populated according to the Boltzmann distribution, and $\rho_r(-\mathcal{T}/2)$ is the product of the density matrices of the individual oscillators [13]. The initial condition on $\rho_{sf}(-\mathcal{T}/2)$ is that it correspond to a Born-Oppenheimer pure state. Thus the slow system is prepared in the position eigenstate $|\mathbf{x}'\rangle$, and the fast system in the negative energy state $|E_-[\mathbf{x}']\rangle$ corresponding to the pseudo-spin aligned along $\mathbf{x}'$ (i. e. $\sigma = 1/2$): $\rho_{sf}(-\mathcal{T}/2) = |\mathbf{x}', 1/2\rangle\langle \mathbf{x}', 1/2| \equiv \tilde{\rho}_{E_-}(-\mathcal{T}/2)$. Thus,

$$\langle \mathbf{x}_f, \sigma_f, \mathbf{Q}_f | \rho(t) | \mathbf{y}_f, \sigma'_f, \mathbf{Z}_f \rangle =$$
$$\int d\mathbf{x}' d\mathbf{y}' d\mathbf{Q}' d\mathbf{Z}'\, \rho_r(\mathbf{Q}', \mathbf{Z}', -\mathcal{T}/2)\, \tilde{\rho}_{E_-}(\mathbf{x}', \mathbf{y}', -\mathcal{T}/2)$$
$$\times\, K(\mathbf{x}_f, \sigma_f, \mathbf{Q}_f, t; \mathbf{x}', 1/2, \mathbf{Q}', -\mathcal{T}/2)\, K^*(\mathbf{y}_f, \sigma'_f, \mathbf{z}_f, t; \mathbf{y}', 1/2, \mathbf{Z}', -\mathcal{T}/2). \quad (13)$$

B. Born-Oppenheimer Treatment of Slow/Fast Dynamics

Implementing the Born-Oppenheimer approximation in Berry phase systems is well-understood [16–18]. We present the analysis for K. A similar analysis applies for K^*, but will not be given here.

K describes evolution over the time interval $[-\mathcal{T}/2, t]$. We introduce intermediate times t_i, $(i = 1, \ldots, N-1)$, and break the evolution into N smaller intervals of duration $\epsilon = (t + \mathcal{T}/2)/N$. Thus,

$$K = \langle \mathbf{x}_f, \sigma_f, \mathbf{Q}_f | \prod_{i=1}^{N} U(t_i, t_{i-1}) | \mathbf{x}', 1/2, \mathbf{Q}' \rangle, \quad (14)$$

with $U(t_i, t_{i-1}) = 1 - i\epsilon H(t_i)/\hbar$. Inserting basis sets $|\mathbf{x}_i, \sigma_i, \mathbf{Q}'_i\rangle \equiv |\mathbf{x}_i\rangle\, |E_{\sigma_i}[\mathbf{x}_i]\,\rangle |\mathbf{Q}'_i\rangle$ at the intermediate times t_i, eqn. (14) breaks up into a product of factors describing evolution over the time intervals $(t_{i-1},\, t_i)$. The factor associated with the i-th time interval is,

$$\langle \mathbf{x}_i, \sigma_i, \mathbf{Q}'_i | \left[1 - \frac{i\epsilon}{\hbar}(H_s + H_{sf} + H_r + H_{sr}) \right] | \mathbf{x}_{i-1}, \sigma_{i-1}, \mathbf{Q}'_{i-1} \rangle$$

$$= \quad \langle \mathbf{x}_i, \mathbf{Q}'_i | \left[\begin{array}{l} \langle\, E_{\sigma_i}[\mathbf{x}_i] | \left(1 - \frac{i\epsilon}{\hbar} H_s\right) | E_{\sigma_{i-1}}[\mathbf{x}_{i-1}] \,\rangle \\ \qquad - \frac{i\epsilon}{\hbar} E_{\sigma_i}[\mathbf{x}_i]\, \delta_{\sigma_i, \sigma_{i-1}} \\ \qquad\quad - \frac{i\epsilon}{\hbar}(H_r + H_{sr}) \delta_{\sigma_i, \sigma_{i-1}} + \mathcal{O}(\epsilon^2) \end{array} \right] | \mathbf{x}_{i-1}, \mathbf{Q}'_{i-1} \rangle \quad (15)$$

Recall that the slow system evolves adiabatically relative to the fast system. Thus the fast system will remain in the initial (negative) energy-level (i. e. $\sigma_i = 1/2$ for all i). Furthermore [6,16–18],

$$\langle\, E_{\sigma_i}[\mathbf{x}_i] | E_{\sigma_{i-1}}[\mathbf{x}_{i-1}] \,\rangle = 1 + i\epsilon\dot{\gamma}_-(t_i) + \mathcal{O}(\epsilon^2),$$

and,

$$\langle\, E_{\sigma_i}[\mathbf{x}_i] |\, H_s \,| E_{\sigma_{i-1}}[\mathbf{x}_{i-1}] \,\rangle = H_{eff}(t_i) + \mathcal{O}(\epsilon^2).$$

Here $\gamma_-(t)$ is the Berry phase associated with the fast system state $|E_-[\mathbf{x}]\,\rangle$, and $H_{eff}(t)$ is given by eqn. (5), with the state appearing in eqns. (6) and (7) given by $|E_-[\mathbf{x}]\,\rangle$.

Inserting all these results into eqn. (14) gives,

$$K = \langle \mathbf{x}_f, \mathbf{Q}_f | \exp\left[-\frac{i}{\hbar} \int_{-\mathcal{T}/2}^{t} d\tau H'(\tau) \right] | \mathbf{x}', \mathbf{Q}' \rangle, \tag{16}$$

where,

$$H'(\tau) = -\hbar\dot{\gamma}_-(\tau) + E_-(\tau) + H_{eff}(\tau).$$

Notice that explicit reference to the fast system has disappeared because the adiabatic time dependence and the initial condition force it to remain in the E_- energy-level at all times. In its place, the back action of the fast system on the slow system has produced the Born-Oppenheimer potential energy $E_-[\mathbf{x}]$, and the gauge potentials $\Phi[\mathbf{x}]$ and $\mathbf{A}[\mathbf{x}]$ in $H'(\tau)$. Equation (16) can be written as a path integral in the usual way [19],

$$K(\mathbf{x}_f, \sigma_f, \mathbf{Q}_f, t; \mathbf{x}', 1/2, \mathbf{Q}', -\mathcal{T}/2) = \delta_{\sigma_f, 1/2} \int \mathcal{D}\mathbf{x}(t) \mathcal{D}\mathbf{Q}(t) \exp\left[\frac{i}{\hbar}(S_s + S_r + S_{sr}) \right]. \tag{17}$$

Here,

$$S_s = \int dt \left[\frac{M}{2}\dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{A}[\mathbf{x}] - \Phi[\mathbf{x}] - E_-[\mathbf{x}] - V[\mathbf{x}] \right], \tag{18}$$

$$S_r = \int dt \sum_j \frac{m_j}{2} \left(\dot{\mathbf{Q}}_j^2 - \omega_j^2 \mathbf{Q}_j^2 \right), \tag{19}$$

$$S_{sr} = \int dt \left[-\sum_j C_j \mathbf{x}_j \cdot \mathbf{Q}_j - \mathbf{x}^2 \sum_j \frac{C_j^2}{2m_j\omega_j^2} \right]. \tag{20}$$

All paths $\mathbf{x}(t)$ ($\mathbf{Q}(t)$) appearing in eqn. (17) begin at $\mathbf{x}'$ ($\mathbf{Q}'$) and end at $\mathbf{x}_f$ ($\mathbf{Q}_f$).

C. Tracing Out the Resevoir

When K and K^* are substituted into eqn. (13), we find,

$$\begin{aligned}\langle \mathbf{x}_f, \sigma_f, \mathbf{Q}_f | \rho(t) | \mathbf{y}_f, \sigma'_f, \mathbf{Z}_f \rangle = \delta_{\sigma_f,1/2}\, \delta_{\sigma'_f,1/2} \\ \times \int d\mathbf{x}' d\mathbf{y}' \tilde{\rho}_{E_-}(\mathbf{x}', \mathbf{y}', -\mathcal{T}/2) \\ \times \int d\mathbf{Q}' d\mathbf{Z}' \rho_r(\mathbf{Q}', \mathbf{Z}', -\mathcal{T}/2) \\ \times \int \mathcal{D}\mathbf{x}(t) \mathcal{D}\mathbf{x}'(t) \mathcal{D}\mathbf{Q}(t) \mathcal{D}\mathbf{Q}'(t) \exp\left[\frac{i}{\hbar}\left(S[\mathbf{x}, \mathbf{Q}] - S[\mathbf{x}', \mathbf{Q}']\right)\right]. \quad (21)\end{aligned}$$

Since the resevoir degrees of freedom are unobserved, we must trace over them. Setting $\mathbf{Q}_f = \mathbf{Z}_f$ in eqn. (21) and integrating over $\mathbf{Q}_f$, the left-hand side (lhs) becomes the reduced density matrix $\tilde{\rho}_{E_-}(\mathbf{x}_f, \mathbf{y}_f, t)$, while the full equation determines its time dependence,

$$\tilde{\rho}_{E_-}(\mathbf{x}_f, \mathbf{y}_f, t) = \int d\mathbf{x}' d\mathbf{y}' J_{E_-}(\mathbf{x}_f, \mathbf{y}_f, t; \mathbf{x}', \mathbf{y}', -\mathcal{T}/2)\, \tilde{\rho}_{E_-}(\mathbf{x}', \mathbf{y}', -\mathcal{T}/2), \quad (22)$$

where,

$$J_{E_-}(\mathbf{x}_f, \mathbf{y}_f, t; \mathbf{x}', \mathbf{y}', -\mathcal{T}/2) = \int \mathcal{D}\mathbf{x}(t) \mathcal{D}\mathbf{x}'(t) \exp\left[\frac{i}{\hbar}\left(S_s[\mathbf{x}] - S_s[\mathbf{x}']\right)\right] \mathcal{F}[\mathbf{x}, \mathbf{x}']. \quad (23)$$

All paths $\mathbf{x}(t)$ ($\mathbf{x}'(t)$) appearing in eqn. (23) begin at $\mathbf{x}'$ ($\mathbf{y}'$) and end at $\mathbf{x}_f$ ($\mathbf{y}_f$). $\mathcal{F}[\mathbf{x}, \mathbf{x}']$ is the influence functional [13] which contains all the effects of the resevoir on the motion of the slow system. For a resevoir composed of harmonic oscillators, $\mathcal{F}[\mathbf{x}, \mathbf{x}']$ can be evaluated exactly [13],

$$\mathcal{F}[\mathbf{x}, \mathbf{x}'] = \exp\left[-\frac{1}{\hbar}\int_{-\mathcal{T}/2}^{t} d\tau ds\, [\mathbf{x}(\tau) - \mathbf{x}'(\tau)]\, [\alpha(\tau - s)\mathbf{x}(s) - \alpha^*(\tau - s)\mathbf{x}'(s)]\right], \quad (24)$$

and $\alpha(\tau - s) = \alpha_R(\tau - s) + i\alpha_I(\tau - s)$ (see below). Thus,

$$\begin{aligned}J_{E_-}(\mathbf{x}_f, \mathbf{y}_f, t; \mathbf{x}', \mathbf{y}', -\mathcal{T}/2) = \int \mathcal{D}\mathbf{x}(t) \mathcal{D}\mathbf{x}'(t) \\ \times \exp\left[\frac{i}{\hbar}\left(S_s[\mathbf{x}] - S_s[\mathbf{x}'] - \int_{-\mathcal{T}/2}^{t} d\tau ds\, [\mathbf{x}(\tau) - \mathbf{x}'(\tau)]\, \alpha_I(\tau - s)\, [\mathbf{x}(s) + \mathbf{x}'(s)]\right)\right] \\ \times \exp\left[-\frac{1}{\hbar}\int_{\mathcal{T}/2}^{t} d\tau ds\, [\mathbf{x}(\tau) - \mathbf{x}'(\tau)]\, \alpha_R(\tau - s)\, [\mathbf{x}(s) - \mathbf{x}'(s)]\right], \quad (25)\end{aligned}$$

where,

$$\alpha_R(\tau - s) = \sum_j \frac{C_j^2}{2m_j\omega_j} \coth\left(\frac{\hbar\omega_j}{2kT}\right) \cos\left[\omega_j(\tau - s)\right] \quad (26)$$

$$\alpha_I(\tau - s) = -\sum_j \frac{C_j^2}{2m_j\omega_j} \sin\left[\omega_j(\tau - s)\right]. \quad (27)$$

Eqns. (25)–(27) give the effective dynamics of the slow system. Geometrical effects have produced gauge fields in $S_s[\mathbf{x}]$; and the stochastic and dissipative effects due to the resevoir lurk in the terms containing α_R and α_I, respectively, though this will not become apparent until we take the semiclassical limit of the effective dynamics.

V. SLOW SYSTEM EFFECTIVE DYNAMICS: SEMICLASSICAL LIMIT

Within the context of our model, we have established the slow system's effective quantum dynamics. In this Section we will see that the semi-classical limit of this dynamics is dissipative and stochastic. This limit is taken in Section V A. In Section V B we obtain the Langevin equation governing the stochastic motion, and the probability distribution functional characterizing the statistical properties of this motion. The Langevin equation is found to contain the same geometric forces that appeared in the deterministic Born-Oppenheimer scenario discussed in Section II.

A. Semiclassical Limit of J_{E_-}

Eqn. (23) describes the slow system effective dynamics. In the absence of a resevoir, the influence functional $\mathcal{F}[\mathbf{x},\mathbf{x}'] = 1$, and the semiclassical limit of the remaining exponential factor can be obtained by the method of steepest descent. When the resevoir is present, $\mathcal{F}[\mathbf{x},\mathbf{x}'] \neq 1$, and we must examine the form it takes when $\hbar \to 0$. For a resevoir composed of harmonic oscillators, this limit has been carried out in Ref. [14]. The result is,

$$\begin{aligned} J^{sc}_{E_-}(\mathbf{x}_f,\mathbf{y}_f,t;\mathbf{x}',\mathbf{y}',-\mathcal{T}/2) &= \int \mathcal{D}\mathbf{x}(t)\mathcal{D}\mathbf{x}'(t) \\ &\quad\times \exp\left[\frac{i}{\hbar}\left(S_s[\mathbf{x}] - S_s[\mathbf{x}'] - \frac{\eta}{2}\int_{-\mathcal{T}/2}^{t} d\tau\ [\mathbf{x}(\tau)-\mathbf{x}'(\tau)]\cdot[\dot{\mathbf{x}}(\tau)+\dot{\mathbf{x}}'(\tau)]\right)\right] \\ &\quad\times \exp\left[-\frac{\eta K T}{\hbar^2}\int_{-\mathcal{T}/2}^{t} d\tau\ \{\mathbf{x}(\tau)-\mathbf{x}'(\tau)\}^2\right] \quad . \end{aligned} \tag{28}$$

The physical significance of η will become clear in Section V B.

The real exponential factor in eqn. (28) introduces important simplifications when $\hbar \to 0$. In this limit, it is very sharply peaked about $\mathbf{x}(\tau) = \mathbf{x}'(\tau)$ so that the dominant contribution to the integral comes from pairs of paths for which $|\mathbf{x}(\tau) - \mathbf{x}'(\tau)| \ll 1$, for all τ. Because the paths $\mathbf{x}(\tau)$ and $\mathbf{x}'(\tau)$ are continuous, $J^{sc}_{E_-}$ is also sharply peaked about $\mathbf{x}_f = \mathbf{y}_f$ and $\mathbf{x}' = \mathbf{y}'$. By eqn. (22), $\rho^{sc}_{E_-}(\mathbf{x},\ \mathbf{y},\ t)$ is similarly sharply peaked about $\mathbf{x} = \mathbf{y}$. Thus, expanding the argument of the complex exponential in eqn. (28) to second order in $[\mathbf{x}(\tau) - \mathbf{x}'(\tau)]$ introduces negligible error when $\hbar \to 0$ [15]. To carry out the expansion, it proves convenient to introduce center-of-mass and relative coordinates, respectively, $\mathbf{R}(\tau)$ and $\boldsymbol{\rho}(\tau)$:

$$\mathbf{R}(\tau) = \frac{\mathbf{x}(\tau)+\mathbf{x}'(\tau)}{2} \qquad ; \qquad \boldsymbol{\rho}(\tau) = \mathbf{x}(\tau) - \mathbf{x}'(\tau) \quad . \tag{29}$$

Using eqn. (18), it is straightforward to show that

$$S_s[\mathbf{x}] - S_s[\mathbf{x}'] = \int_{-\mathcal{T}/2}^{t} d\tau\ \left[\boldsymbol{\rho}(\tau)\cdot\left(-M\ddot{\mathbf{R}} + \dot{\mathbf{R}}\times\mathbf{B}[\mathbf{R}] + \mathbf{E}[\mathbf{R}]\right) + \mathcal{O}\left(|\boldsymbol{\rho}|^3\right)\right] . \tag{30}$$

Here $\mathbf{B}[\mathbf{R}] = \nabla\times\mathbf{A}[\mathbf{R}]$; $\mathbf{E}[\mathbf{R}] = -\nabla\left(\Phi[\mathbf{R}] + V[\mathbf{R}] + E_-[\mathbf{R}]\right)$; and $\mathbf{A}[\mathbf{R}]$ and $\Phi[\mathbf{R}]$ are the geometric gauge potentials discussed in Section II. It follows immediately from eqn. (29) that,

$$-\frac{\eta}{2}\int_{-\mathcal{T}/2}^{t} d\tau\ [\mathbf{x}(\tau)-\mathbf{x}'(\tau)]\cdot[\dot{\mathbf{x}}(\tau)+\dot{\mathbf{x}}'(\tau)] = -\eta\int_{-\mathcal{T}/2}^{t} d\tau\ \boldsymbol{\rho}(\tau)\cdot\dot{\mathbf{R}}(\tau). \tag{31}$$

Putting together all these results gives,

$$\begin{aligned} J_{E_-}^{sc}(\mathbf{x}_f,\mathbf{y}_f,t;\mathbf{x}',\mathbf{y}',-\mathcal{T}/2) = \int \mathcal{D}\mathbf{R}(t)\mathcal{D}\boldsymbol{\rho}(t) \\ \times \exp\left[\frac{i}{\hbar}\int_{-\mathcal{T}/2}^{t} d\tau\boldsymbol{\rho}(\tau)\cdot\left[-M\ddot{\mathbf{R}}-\eta\dot{\mathbf{R}}+\dot{\mathbf{R}}\times\mathbf{B}+\mathbf{E}\right]\right] \\ \times \exp\left[-\frac{\eta kT}{\hbar^2}\int_{-\mathcal{T}/2}^{t} d\tau\,[\boldsymbol{\rho}(\tau)]^2\right]. \end{aligned} \tag{32}$$

B. Appearance of Stochastic Dynamics

To bring out the stochastic character of the dynamics contained in eqn. (32), we again focus on the real exponential in this equation. Its argument can be re-written as,

$$-\frac{\eta kT}{\hbar^2}\int_{-\mathcal{T}/2}^{t} d\tau\boldsymbol{\rho}(\tau)\cdot\boldsymbol{\rho}(\tau) = -\frac{1}{2\hbar^2}\int_{-\mathcal{T}/2}^{t}\int_{-\mathcal{T}/2}^{t} d\tau ds\ \rho_i(\tau)A_{ij}(\tau-s)\rho_j(s), \tag{33}$$

where $A_{ij}(\tau-s) = 2\eta kT\delta_{ij}\delta(\tau-s)$. To bring out the meaning of this term we introduce a Hubbard-Stratonovitch transformation:

$$\begin{aligned} \Phi[\boldsymbol{\rho}] &\equiv \exp\left[-\frac{1}{2\hbar^2}\int_{-\mathcal{T}/2}^{t}\int_{-\mathcal{T}/2}^{t} d\tau ds\rho_i(\tau)A_{ij}(\tau-s)\rho_j(s)\right] \\ &= \frac{1}{N}\int \mathcal{D}\mathbf{F}(t)\exp\left[-\frac{1}{2}\int_{-\mathcal{T}/2}^{t}\int_{-\mathcal{T}/2}^{t} d\tau dsF_i(\tau)A_{ij}^{-1}(\tau-s)F_j(s)\right] \\ &\qquad \times\exp\left[\frac{i}{\hbar}\int_{-\mathcal{T}/2}^{t} d\tau\boldsymbol{\rho}(\tau)\cdot\mathbf{F}(\tau)\right], \end{aligned} \tag{34}$$

where $A_{ij}^{-1}(\tau-s) = (1/2\eta kT)\delta_{ij}\delta(\tau-s)$, and N is an (infinite) normalization constant which we suppress below. Eqn. (34) is an identity which can be proved by evaluating the Gaussian integral on the rhs. From eqn. (34), it is clear that $\Phi[\boldsymbol{\rho}]$ is the characteristic functional for the Gaussian random process $\mathbf{F}(t)$. Functional derivatives of $\Phi[\boldsymbol{\rho}]$ with respect to $\boldsymbol{\rho}(t)$ generate the correlation functions of $\mathbf{F}(t)$. In particular,

$$\langle F_i(\tau)F_j(s)\rangle = \left(\frac{\hbar}{i}\right)^2\frac{\delta^2\Phi[\boldsymbol{\rho}]}{\delta\rho_i(\tau)\delta\rho_j(s)} = A_{ij}(\tau-s) = 2\eta kT\delta_{ij}\delta(\tau-s). \tag{35}$$

Thus $\mathbf{F}(t)$ has a two-point correlation function identical to that of a classical stochastic force produced by a heat resevoir with friction coefficient η and temperature T. We shall see below that this is the correct interpretation for $\mathbf{F}(t)$.

Making use of eqn. (34) in eqn. (32) gives,

$$\begin{aligned} J_{E_-}^{sc}(\mathbf{x}_f,\mathbf{y}_f,t;\mathbf{x}',\mathbf{y}',-\mathcal{T}/2) = \int \mathcal{D}\mathbf{R}(t)\mathcal{D}\boldsymbol{\rho}(t)\mathcal{D}\mathbf{F}(t) \\ \times\exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{t} d\tau\,[\mathbf{F}(\tau)]^2\right]\exp\left[\frac{i}{\hbar}\int_{-\mathcal{T}/2}^{t} d\tau\boldsymbol{\rho}(\tau)\cdot\hat{L}\mathbf{R}(\tau)\right], \end{aligned} \tag{36}$$

where $\hat{L}\mathbf{R}(\tau) \equiv -M\ddot{\mathbf{R}} - \eta\dot{\mathbf{R}} + \dot{\mathbf{R}} \times \mathbf{B} + \mathbf{E}$. We recognize the $\boldsymbol{\rho}(t)$-integral as the Dirac delta functional. Thus,

$$J^{sc}_{E_-}(\mathbf{x}_f, \mathbf{y}_f, t; \mathbf{x}', \mathbf{y}', -\mathcal{T}/2) = \int \mathcal{D}\mathbf{R}(t)\mathcal{D}\mathbf{F}(t) \\ \times \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{t} d\tau\, [\mathbf{F}(\tau)]^2\right] \delta\left[\hat{L}\mathbf{R}(t) + \mathbf{F}(t)\right]. \quad (37)$$

Clearly, in the semiclassical limit, the only paths that contribute to $J^{sc}_{E_-}$ are those which satisfy the Langevin equation,

$$\hat{L}\mathbf{R}(t) + \mathbf{F}(t) = 0, \quad (38)$$

or,

$$M\ddot{\mathbf{R}} = -\eta\dot{\mathbf{R}} + \dot{\mathbf{R}} \times \mathbf{B}[\mathbf{R}] + \mathbf{E}[\mathbf{R}] + \mathbf{F}(t). \quad (39)$$

As promised in Section III, introducing the resevoir has caused the semiclassical dynamics of the slow system to become stochastic. η can be interpreted as a friction coefficient, and $\mathbf{F}(t)$ as a Gaussian stochastic force. We also see that the geometric Lorentz-like and electric-like forces which appear in the deterministic Born-Oppenheimer scenario (see eqn. (8)) also appear in the (adiabatic) stochastic generalization of this scenario. Eqn. (39) corresponds to one of the two main results of this Section.

To obtain the second, we carry out the $\mathbf{F}(t)$-integration,

$$J^{sc}_{E_-}(\mathbf{R}_f, \boldsymbol{\rho}_f = 0, t; \mathbf{R}', \boldsymbol{\rho}' = 0, -\mathcal{T}/2) = \int \mathcal{D}\mathbf{R}(t) \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{t} d\tau \left[\hat{L}\mathbf{R}(\tau)\right]^2\right]. \quad (40)$$

Inserting this into eqn. (22), we find,

$$\rho^{sc}_{E_-}(\mathbf{R}_f, \boldsymbol{\rho}_f = 0, t) = \\ \int d\mathbf{R}' \int \mathcal{D}\mathbf{R}(t) \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{t} d\tau \left[\hat{L}\mathbf{R}(\tau)\right]^2\right] \rho^{sc}_{E_-}(\mathbf{R}', \boldsymbol{\rho}' = 0, -\mathcal{T}/2). \quad (41)$$

We see that $\rho^{sc}_{E_-}(\mathbf{R}_f, t)$ is found by summing over all paths which lead from $\mathbf{R}'$ to $\mathbf{R}_f$, and then integrating over all possible $\mathbf{R}'$. From eqn. (41), the probability that a path $\mathbf{R}(t)$ lies in a "volume" $\mathcal{D}\mathbf{R}(t)$ in the space of paths that join $\mathbf{R}'$ to $\mathbf{R}_f$ is clearly,

$$\mathcal{D}P = \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{t} d\tau \left[\hat{L}\mathbf{R}(\tau)\right]^2\right] \mathcal{D}\mathbf{R}(t). \quad (42)$$

This identifies the probability distribution functional $P[\mathbf{R}(t)]$ as,

$$P[\mathbf{R}(t)] = \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{t} d\tau \left[\hat{L}\mathbf{R}(\tau)\right]^2\right]. \quad (43)$$

We will use eqn. (43) in the following section to calculate the average shift and broadening of the fast system energy-levels.

VI. FAST SYSTEM ENERGY LEVEL-SHIFT AND BROADENING

In this Section we calculate approximately the average shift and broadening produced in the fast system energy levels by the combination of Berry phase and stochastic effects. In Section VI A, we introduce the generating function that is the basis of our calculation, and state the conditions we must impose to make the calculation tractable. The generating function is evaluated in Section VI B. In Section VI C and VI D, we determine the approximate average level-shift and level-broadening, respectively.

A. Preliminaries

We restrict the slow system to two-spatial dimensions: $\mathbf{R}(t) = R(t)[\cos\phi(t),\ \sin\phi(t), 0]$. H_{sf} takes the form:

$$H_{sf} = gR(t)\begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}.$$

We assume throughout this Section that the fast system is initially prepared in the state $|E_{-}[\mathbf{R}_i]\,\rangle$, where $\mathbf{R}(-\mathcal{T}/2) \equiv \mathbf{R}_i$. Using eqns. (6) and (7),

$$\Phi_{-}[\mathbf{R}] = \frac{(\hbar\nabla\phi)^2}{2M} = \frac{\hbar^2}{2MR^2} \qquad ; \qquad \mathbf{A}[\mathbf{R}] = -\frac{\hbar\nabla\phi}{2} = \frac{\hbar}{2R^2}\mathbf{R}\times\hat{\mathbf{z}}. \tag{44}$$

From these, $\mathbf{B} = \nabla\times\mathbf{A}$, and $\mathbf{E} = -\nabla(\Phi_{-}[\mathbf{R}] + V[\mathbf{R}] + E_{-}[\mathbf{R}])$. To simplify the following calculation, we choose $V[\mathbf{R}] = -E_{-}[\mathbf{R}]$.

Our Langevin equation becomes,

$$M\ddot{\mathbf{R}} = -\eta\dot{\mathbf{R}} - \frac{h}{2}\delta^2(\mathbf{R})\dot{\mathbf{R}}\times\hat{\mathbf{z}} + \frac{h^2}{MR^3}\hat{\mathbf{R}} + \mathbf{F}(t). \tag{45}$$

The Lorentz force is seen to vanish everywhere except at the origin, while the electric force is divergent there and repulsive. Consequently, any finite energy motion of the slow system must have a turning point with $R_{tp} \neq 0$. In 2D, then, the Lorentz force disappears from eqn. (45). The electric force is seen to cut off rather quickly, and is second order in Planck's constant h. Thus, away from the origin, the electric force is small in the semiclassical limit. To simplify the following analysis, we replace the exact electric force with something qualitatively similar. To capture the strong repulsion at the origin, we simply remove the origin from the xy-plane so that $R(t) \neq 0$ for all t. To mimic the rapid cutoff away from the origin, we simply drop the electric force from eqn. (45). With this simplification, our Langevin equation reduces to free Brownian motion in the punctured xy-plane:

$$\hat{L}\mathbf{R} = M\ddot{\mathbf{R}} + \eta\dot{\mathbf{R}} = \mathbf{F}. \tag{46}$$

The boundary conditions are: $\mathbf{R}(-\mathcal{T}/2) = \mathbf{R}_i$, and $\mathbf{R}(\mathcal{T}/2) = \mathbf{R}_f$.

We write $\mathbf{R}(t) = \mathbf{R}_0(t) + \mathbf{y}(t)$. Here $\mathbf{R}_0(t)$ is the homogeneous solution of eqn. (46); and $\mathbf{y}(t)$ is a particular solution. $\mathbf{R}_0(t)$ satisfies the same boundary conditions as $\mathbf{R}(t)$, so consequently, $\mathbf{y}(\pm\mathcal{T}/2) = 0$. We want a condition that insures that the fluctuating particular

solution $\mathbf{y}(t)$ remains small compared to the noiseless homogeneous solution $\mathbf{R}_0(t)$ in an average sense: $\langle|\mathbf{y}(t)|^2\rangle \ll |\mathbf{R}_0(t)|^2$. For Brownian motion, it is well-known that [20],

$$\langle|\mathbf{y}(t)|^2\rangle \sim \frac{2kT}{\eta}t. \tag{47}$$

Defining $\overline{\mathbf{R}} = (\mathbf{R}_i + \mathbf{R}_f)/2$; requiring $\langle|\mathbf{y}(t)|^2\rangle \ll \overline{R}^2$; and using eqn. (47) gives the condition we seek,

$$kT \ll \frac{\eta\overline{R}^2}{\mathcal{T}}. \tag{48}$$

Brownian motion which satisfies eqn. (48) will be referred to as low-noise Brownian motion.

The central object of this Section is the generating function $F(\rho)$ for the moments of the energy-level shifts $\delta E_{-}[\mathbf{R}]$ (see eqn. (3)):

$$F(\rho) = \int \mathcal{D}\mathbf{R}(t)\, P[\mathbf{R}] \exp[\rho\delta E[\mathbf{R}]]. \tag{49}$$

It follows immediately that,

$$\left.\frac{d[\ln F(\rho)]}{d\rho}\right|_{\rho=0} = \frac{\int \mathcal{D}\mathbf{R}(t)\, P[\mathbf{R}]\delta E[\mathbf{R}]}{\int \mathcal{D}\mathbf{R}(t)\, P[\mathbf{R}]} = \overline{\delta E}, \tag{50}$$

and,

$$\frac{d^2[\ln F(\rho)]}{d\rho^2}\,|_{\rho=0} = \overline{(\delta E)^2} - (\overline{\delta E})^2 = \sigma^2. \tag{51}$$

We will use the standard deviation σ as a measure of the energy-level broadening.

B. Generating Function

Using eqns. (2), (3), (6), (43), (44), and (49) gives,

$$F(\rho) = \int \mathcal{D}\mathbf{R}(t)\, \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{\mathcal{T}/2} d\tau\, \left\{(\hat{L}\mathbf{R})^2 + e\rho\,\hat{\mathbf{z}}\cdot\dot{\mathbf{R}}\times\mathbf{R}/R^2\right\}\right], \tag{52}$$

where $e = -2\eta kT\hbar/\mathcal{T}$. It is not possible to evaluate eqn. (52) analytically under arbitrary conditions. The calculation is analytically tractable if we restrict ourselves to low-noise Brownian motion. As discussed in Section VI A, in the low-noise limit, the fluctuating component $\mathbf{y}(t)$ is always small compared to the noiseless component $\mathbf{R}_0(t)$.This allows us to expand the argument A of the exponential in eqn. (52) to second-order in $\mathbf{y}(t)$, yielding a Gaussian path integral. The presence of R^2 in the denominator of the second term appearing in the integrand of A complicates the analysis however. Since the noise component $\mathbf{y}(t)$ is small, $R^2 \approx \overline{R}^2$ throughout the motion. Consequently, we will approximate R^2 by $\overline{R}^2$ in this denominator. Strictly speaking, we are discarding terms that should be kept by doing this. As such, our results in Section VI C and VI D should be thought of more as rough estimates,

than as rigorous results (see the discussion at the end of Section VI D). In principle, one could repeat the calculation below including these extra terms, though we will not do so here. Carrying out this expansion gives,

$$F(\rho) = \exp\left[\rho\delta E_{-}[\mathbf{R}_0]\right] \int \mathcal{D}\mathbf{y}(t)\, \exp\left[-\frac{1}{4\eta kT}\int_{-\mathcal{T}/2}^{\mathcal{T}/2} d\tau\, I[\mathbf{y}]\right]. \tag{53}$$

Here,

$$I[\mathbf{y}] = \left[M^2(\ddot{\mathbf{y}})^2 + \eta^2(\dot{\mathbf{y}})^2 + 2M\eta\,\dot{\mathbf{y}}\cdot\ddot{\mathbf{y}}\right] + \frac{e\rho\epsilon^{3ij}}{\overline{R}^2}\left[2\dot{R}_0^i\, y_j + \dot{y}_i\, y_j\right], \tag{54}$$

and ϵ^{ijk} is the Levi-Civita density.

It proves useful to Fourier transform $\mathbf{y}(t)$. A sine-transform is needed since $\mathbf{y}(\pm\mathcal{T}/2) = 0$,

$$\mathbf{y}(t) = \sum_{n=1}^{n_b} \mathbf{y}_n \sin\left(\frac{n\pi}{\mathcal{T}}t\right).$$

The need for adiabatic noise requires an upper cutoff $\omega_b = n_b\pi/\mathcal{T}$ on the noise spectrum (see Section III). The boundary conditions produce a low frequency cutoff $\omega_c = \pi/\mathcal{T}$. We assume $\mathcal{T}$ is large, though finite, so that $\mathbf{y}(t)$ can be written as a complex Fourier integral,

$$\mathbf{y}(t) = \frac{1}{2\pi}\int_{-\omega_b}^{\omega_b} d\omega\, \mathbf{y}(\omega)\exp[-i\omega t], \tag{55}$$

where continuation to negative ω requires $\mathbf{y}(-\omega) = -\mathbf{y}(\omega)$. Note that this is consistent with the boundary condition requirement that there be no zero-frequency mode in the noise spectrum. Substituting eqn. (55) into eqn. (53), and completing the square in the integrand gives (eventually),

$$\begin{aligned} F(\rho) = \exp&\left[\rho\delta E_{-}[\mathbf{R}_0] + \frac{1}{4\eta kT}\int_{-\omega_b}^{\omega_b}\frac{d\omega}{2\pi} B_i^*(\omega) A_{ij}^{-1}(\omega) B_j(\omega)\right] \\ &\times \int \mathcal{D}\mathbf{z}(\omega)\exp\left[-\frac{1}{4\eta kT}\int_{-\omega_b}^{\omega_b}\frac{d\omega}{2\pi} z_i^*(\omega) A_{ij}(\omega) z_j(\omega)\right], \end{aligned} \tag{56}$$

where,

$$A_{ij}(\omega) = \delta_{ij}\left(M^2\omega^4 + \eta^2\omega^2\right) + \epsilon^{3ij}\left(\frac{i\omega e\rho}{\overline{R}^2}\right); \tag{57}$$

$$B_j(\omega) = \frac{e\rho\epsilon^{3ij}}{\overline{R}^2}\left(-i\omega R_0^i(\omega)\right). \tag{58}$$

Carrying out the Gaussian integral gives,

$$F(\rho) = \frac{Y(\rho)}{X(\rho)}, \tag{59}$$

where,

$$Y(\rho) = \exp\left[c_1\rho + \frac{c_2\rho^2}{2}\int_{-\omega_b}^{\omega_b}\frac{d\omega}{2\pi}\omega^2\left\{\frac{f_1-\rho f_2}{f_3-\rho^2 f_4}\right\}\right], \tag{60}$$

$$X(\rho) = \sqrt{\prod_\omega c_3(f_3-\rho^2 f_4)}, \tag{61}$$

and,

$$\begin{array}{lcl} c_1 = \delta E_-[\mathbf{R}_0] & ; & f_1 = |\mathbf{R}_0(\omega)|^2(M^2\omega^4+\eta^2\omega^2) \\ c_2 = \eta kT\hbar^2/\mathcal{T}^2\overline{R}^4 & ; & f_2 = i\omega\,[\hat{\mathbf{z}}\cdot\mathbf{R}_0(\omega)\times\mathbf{R}_0^*(\omega)](\eta kT\hbar/\mathcal{T}\overline{R}^2) \\ c_3 = M\overline{R}^2/2\eta^2 kT & ; & f_3 = (M^2\omega^4+\eta^2\omega^2)^2 \\ & & f_4 = (\eta kT\hbar\omega/\mathcal{T}\overline{R}^2)^2. \end{array} \tag{62}$$

C. Average Energy-Level Shift

From eqn. (50),

$$\begin{aligned}\overline{\delta E_-} &= \frac{d}{d\rho}[\ln Y(\rho)]\,|_{\rho=0} - \frac{d}{d\rho}[\ln X(\rho)]\,|_{\rho=0} \\ &= c_1 - 0 \\ &= \delta E_-[\mathbf{R}_0].\end{aligned} \tag{63}$$

In the low-noise limit we find that the average energy-level shift is given by the shift produced by the noiseless component of $\mathbf{R}(t)$. The absence of a further noise correction to eqn. (63) is surely a consequence of the low-noise approximation. Such a noise correction is expected to occur for stronger noise.

D. Average Energy-Level Broadening

From eqn. (51),

$$\begin{aligned}\sigma^2 &= \frac{d^2}{d\rho^2}[\ln Y(\rho)]\,|_{\rho=0} - \frac{d^2}{d\rho^2}[\ln X(\rho)]\,|_{\rho=0} \\ &= c_2\int_{\omega_c}^{\omega_b}\frac{d\omega}{\pi}\frac{\omega^2 f_1}{f_3} + \mathcal{T}\int_{\omega_c}^{\omega_b}\frac{d\omega}{\pi}\frac{f_4}{f_3}.\end{aligned} \tag{64}$$

Solving the homogeneous Langevin equation for $\mathbf{R}_0(t)$, and Fourier transforming to obtain $\mathbf{R}_0(\omega)$; introducing a dimensionless frequency $x = \omega(M/\eta)$; and using eqn. (62) gives (eventually),

$$\sigma = \frac{\hbar}{\mathcal{T}}\sqrt{\left(\frac{MkT}{\eta^2\overline{R}^2}\right)\left[\frac{|\mathbf{R}_f-\mathbf{R}_i|^2}{\overline{R}^2} + \frac{kT}{(\eta\overline{R}^2/\mathcal{T})}\right]\int_{x_c}^{x_b}\frac{dx}{\pi}\frac{1}{x^2(1+x^2)^2}}. \tag{65}$$

A simpler relation can be found if we choose boundary conditions such that,

$$|\mathbf{R}_f - \mathbf{R}_i|^2 \sim \frac{2kT}{\eta}\mathcal{T},$$

which corresponds to fixing the separation of boundary points to be roughly the same size as the diffusion cloud for Brownian motion over a time $\mathcal{T}$. Eqn. (65) becomes,

$$\sigma \sim kT \left(\frac{\hbar}{\eta \overline{R}^2} \right) \kappa, \tag{66}$$

where,

$$\kappa = \sqrt{\frac{3\tau}{\mathcal{T}} \int_{x_c}^{x_b} \frac{dx}{\pi} \frac{1}{x^2(1+x^2)^2}},$$

and $\tau = M/\eta$. As mentioned above, eqns. (65) and (66) should be thought of more as rough estimates, than as rigorous results. Clearly though, we do see that level-broadening is produced by the combination of Berry phase and stochastic effects. A Monte Carlo evaluation of the path integrals appearing in eqns. (50) and (51) would be very interesting since such a calculation would not require the simplifications we found it necessary to make to produce an analytically tractable calculation. It is important to keep in mind that such a Monte Carlo calculation must still satisfy the third condition imposed in Section III to insure that the noise respects the adiabatic requirements of Berry's phase.

VII. CLOSING REMARKS

In the usual Berry phase scenario one considers a pair of interacting systems with vastly different dynamical time scales, and treats the coupled dynamics using the Born-Oppenheimer approximation. In this paper we generalize this scenario, allowing the slow system dynamics to be stochastic as well as adiabatic. We introduce a model that allows us to study how the usual Berry phase scenario is modified by the stochastic dynamics.

Our principal results are: (1) a broadening and shifting of the fast system energy-levels by a combination of Berry phase and stochastic effects; and (2) the semiclassical limit of the slow system effective dynamics obeys a Langevin equation in which geometrical effects produce Lorentz-like and electric-like forces.

In the semiclassical and low-noise limit, we calculate approximately the average level-shift and broadening produced by this geometric mechanism. Monte Carlo evaluation of eqns. (50) and (51) would be very interesting as this would free the analysis from the low-noise limit.

Formally, the semiclassical limit was taken by letting $\hbar \to 0$. In fact, $\hbar$ is finite, and an experimental realization of this limit must be approached differently. Formally, the semiclassical limit is controlled by the real exponential factor appearing in eqn. (28), and is approached when it becomes sharply peaked. This occurs when $\hbar \to 0$, though more generally when $\eta \overline{R}^2 kT\mathcal{T} \gg \hbar^2$. Thus strong damping is one way to produce semiclassical behavior. The low-noise limit required $kT \ll \eta \overline{R}^2/\mathcal{T}$. Thus, sufficiently low temperature will produce low-noise behavior. Our approximate results for the average level-shift and broadening are thus expected to apply in the limit of strong damping and sufficiently low temperature.

In an interesting Comment, Simon and Kumar [21] propose a physical setting in which Berry's phase should produce level-broadening. Their underlying idea is similar to the one we propose: a range of level-shifts occur producing a broadening of the original energy level. They do not provide a formal development of their proposal, however. Gamliel and Reed [22] consider the original Berry phase scenario of a pseudo-spin (fast system) interacting with an adiabatically evolving pseudo-magnetic field (slow system). However, they allow for the presence of a stochastic process whose sole effect is to relax the pseudo-spin to an equilibrium state (which might evolve with time). The stochastic process is assumed to produce *no* Berry phase effects in the pseudo-spin dynamics. The deterministic motion of the pseudo-magnetic field produces a unique level-shift $\delta E[\mathbf{R}]$ in each fast system energy level E. The central question for these authors is whether the shift $\delta E[\mathbf{R}]$ is observable in the presence of the conventional level-broadening produced by the relaxation process. In our scenario, the slow system motion is the random process, and the level-broadening arises through the Berry phase induced level-shifts.

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APPENDIX:

In this Appendix we consider a free classical Brownian particle moving in one-spatial dimension. We will establish a condition that insures that the Brownian motion is adiabatic relative to a quantum system that interacts with the Brownian particle.

The Brownian motion is described by Langevin's equation,

$$m\ddot{R} + \eta\dot{R} = F(t), \tag{A1}$$

where m is the particle mass; η is the friction coefficient; and $F(t)$ is a stochastic force with correlation function,

$$\langle\, F(t)F(t')\,\rangle = 2\eta kT\delta(t-t') \quad . \tag{A2}$$

The stochastic force $F(t)$ fluctuates rapidly. The duration τ_c of a force fluctuation is known as the correlation time. It is determined by the time scale of the microscopic processes which produce the stochastic force. The particle velocity $\dot{R}$ varies on a much slower time scale due to the large inertia of the Brownian particle.

Since the Brownian particle is free, $E = mv^2/2$. The time-averaged energy is

$$\langle\, E\,\rangle = \frac{m}{2}\langle\, v^2\,\rangle = \frac{m}{2}K_v(0),$$

where $K_v(t) = \langle\, v(0)v(t)\,\rangle$ is the velocity correlation function. Its Fourier transform is the spectral density $J_v(\omega)$ of $v(t)$ [23],

$$K_v(t) = \int_0^\infty d\omega \, \cos\omega t \, J_v(\omega) \quad .$$

Thus,

$$\langle E \rangle = \frac{m}{2} \int_0^\infty d\omega \, J_v(\omega) \quad . \tag{A3}$$

Defining the energy spectral density $\rho_E(\omega)$ as the mean noise-energy in the frequency range $(\omega,\, \omega + d\omega)$, we see from eqn. (A3) that,

$$\rho_E(\omega) = \frac{m}{2} J_v(\omega) \quad . \tag{A4}$$

It is well-known [23] that, $J_v(\omega) = \lim_{\mathcal{T}\to\infty} 2|v(\omega)|^2/\mathcal{T}$. Since $v(\omega) = -i\omega R(\omega)$, eqn. (A4) becomes,

$$\rho_E(\omega) = \frac{m\omega^2}{2} J_R(\omega) \quad , \tag{A5}$$

where $J_R(\omega) = \lim_{\mathcal{T}\to\infty} 2|R(\omega)|^2/\mathcal{T}$.

It is preferable to express $\rho_E(\omega)$ in terms of $J_F(\omega)$. To do this we use the Langevin equation to relate $J_R(\omega)$ to $J_F(\omega)$. Fourier transforming eqn. (A1) gives,

$$R(\omega) = \frac{-F(\omega)}{m\omega\,(\omega + i\omega_r)} \quad ,$$

where $\omega_r = \eta/m$. Thus,

$$J_R(\omega) = \frac{J_F(\omega)}{m^2\omega^2(\omega^2 + \omega_r^2)} \quad ,$$

and,

$$\rho_E(\omega) = \frac{J_F(\omega)}{2m\,(\omega^2 + \omega_r^2)} \quad .$$

In writing the force correlation function in eqn. (A2) as being proportional to $\delta(t - t')$, we assumed τ_c was effectively zero, and $J_F(\omega) = 2\eta kT$ for all ω. In fact, τ_c is not zero, though macroscopically small. Thus $J_F(\omega) = 2\eta kT$ only up to a cutoff frequency $\Lambda \sim 1/\tau_c$ so that

$$\rho_E(\omega) = \frac{\eta kT}{m\,(\omega^2 + \omega_r^2)} \Theta(\Lambda - \omega) \quad , \tag{A6}$$

where $\Theta(x)$ vanishes if $x < 0$ and is 1 otherwise. From eqns. (A3)—(A5), and (A6) we see that noise fluctuations in the random process $R(t)$ only exist for frequencies $\omega \leq 1/\tau_c$. If the Brownian particle is coupled to a quantum system whose energy-level spacing is ΔE, the Brownian motion will be unable to produce transitions in the quantum system if $\hbar/\tau_c \ll \Delta E$. If this condition is satisfied, the quantum system will see the Brownian motion as adiabatic. This is the desired adiabaticity condition.

REFERENCES

[1] A. Shapere and F. Wilczek, *Geometric Phases in Physics* (World Scientific, New Jersey, 1989).
[2] M. V. Berry, Proc. R. Soc. Lond. A **392**, 45 (1984).
[3] B. Simon, Phys. Rev. Lett. **51**, 2167 (1983).
[4] J. Moody, A. Shapere, and F. Wilczek, Phys. Rev. Lett. **56**, 893 (1986).
[5] D. Suter, G. C. Chingas, R. A. Harris, and A. Pines, Mol. Phys. **61**, 1327 (1987).
[6] M. V. Berry, in Ref. [1], pp. 7-28.
[7] C. A. Mead and D. G. Truhlar, J. Chem. Phys. **70(05)**, 2284 (1979).
[8] R. Jackiw, Comm. At. Mol. Phys. **20**, 71 (1988).
[9] C. A. Mead, Chem. Phys. **49**, 23 (1980); **49**, 33 (1980).
[10] B. Zygelman, Phys. Lett. A **125**, 476 (1987).
[11] J. P. Provost and G. Vallee, Comm. Math. Phys. **76**, 289 (1980).
[12] A. O. Caldeira and A. J. Leggett, Ann. Phys. **149**, 374 (1983); Errata, Ann. Phys. **153**, 445 (1984).
[13] R. P. Feynman and F. L. Vernon, Ann. Phys. **24**, 118 (1963).
[14] A. O. Caldeira and A. J. Leggett, Physica A **121**, 587 (1983).
[15] A. Schmid, Jour. Low Temp. Phys. **49**, 609 (1982).
[16] M. V. Berry and J. M. Robbins, Proc. R. Soc. Lond. A **442**, 641 (1993).
[17] H. Kuratsuji and S. Iida, Prog. Theor. Phys. **74**, 439 (1985).
[18] F. Gaitan, Phys. Rev. B **51**, 9061 (1995).
[19] L. S. Schulman, *Techniques and Applications of Path Integrals* (John Wiley and Sons, New York, 1981).
[20] A. Einstein, Ann. Phys. (Lpz.) **17**, 549 (1905).
[21] R. Simon and N. Kumar, J. Phys. A **21**, 1725 (1988).
[22] D. Gamliel and J. H. Freed, Phys. Rev. A **39**, 3238 (1989).
[23] M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. **17**, 323 (1945).